## 3D Multiple-point Statistics Simulations of the Roussillon Continental Pliocene Aquifer using DeeSse (Valentin Dall'alba et al)

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## Anonymous Referee #2 (25 May 2020) :

## Specific comments :

1. The starting point for the proposed strategy, as stated in the abstract, is a conceptual model. The conceptual model is considered to be known deterministically. There is no mention of alternative, conceptual models. This is not trivial, and the authors need to justify this approach and suggest how to relax the constraint imposed by using a single conceptual model (see abstract lines 3-5).	We thank the reviewer for pointing out this issue in the abstract. We revised it to mention the possibility of using several alternative training images and conceptual models. Later, in the paper, we already considered three alternative training images (see figure 2), illustrating exactly this point. More conceptual models can be easily included in the workflow and tested.
2. The strategy presented here is smart in that it assimilates concepts from geology with geostatistical concepts. For example, the use of a physical-mathematical model for establishing the spatial evolution of sedimentary patterns. But some additional work is needed.	We thank the reviewer for his positive comment. Just to be sure to be well understood. The physical model that we solve is used only to get the main trends and obtain plausible patterns. We do not solve the complete coupled system of equations describing the whole processes of sediment transport, deposition, compaction, diagenesis, etc. Our approach is very much simplified as compared to proper sedimentary basin modeling approaches.
3. I recall some work done along this line (Item 2 above) by Steve Gorelick's group. As I recall, it requires using weather patterns over geological time scales, for boundary conditions. So, different patterns would have a strong effect on the patterns mentioned in (2).	As we indicate above, we do not model all the processes. We just compute a trend map to control the position of the different types of sedimentary structures in the basin. And then we rely on the multiple-point statistics approach to generate the set of realizations. This is much faster than solving the physical problem and it does not require to provide detailed initial and boundary conditions. Our approach is much simpler but it allows us to generate easily a set of realizations and get some ideas about the uncertainty while the approach based on solving the physics is much more computationally demanding. In addition, the process-based the

	approach is not able to ensure that all the borehole data are honored. Therefore the two methods are very different and complementary.
I am trying to figure out how climate/weather conditions permeated into the modeling of sedimentary patterns. There is a brief and incomplete description of the solution of the diffusivity equation. Just a couple of lines, between Line 170 and Line 175, on the topic. The authors need to shed more light on this aspect of their approach, and to show how the math/physical model used in support of (2) is actually constructed.	As explained above, we do not account for these aspects since we want to model the system in a reasonable manner while remaining as simple as possible.
4. Line 65: Listing the advantages of the a 2010 simulation model, the authors state "no probability is computed". Question is: why is that an advantage? What are the positive and negative implications or avoiding probabilistic models?	It is true that we do not explain this aspect in detail in the paper for the sake of brevity. As explained in detail in the original paper from 2010, the direct sampling technique is a multiple-point statistics (MPS) algorithm that resamples some patterns from the training image in a stochastic manner without computing probabilities. Other MPS algorithms need to estimate the probabilities of the different patterns to produce simulations. Often, this is a problem because to estimate a probability one has to count all possible configurations and check the ones that are compatible with the data. The number of configurations can become extremely large and counting all these different configurations can become a technical limitation in terms of computing time or memory usage. Here, with the direct sampling, we resample some patterns in a manner that we ensure that the probabilities are honored but we do not compute them explicitly. This allows us to consider much more complex situations (more sedimentary facies for example, larger size of the patterns, or multivariate patterns) than more traditional MPS algorithms such as SNESIM. All the tests that we have done since 2010 show that this feature is an important advantage as compared to the other MPS methods because it offers much more flexibility. One possible limitation is that the time required to generate a simulation can be larger if the code is not optimized and parallelized. But this is not the case for DeeSse.

	To avoid entering into a long discussion, we have added some additional references describing some features of the DeeSse algorithm. "In this work, we use the direct sampling algorithm implemented in the DeeSse code (Straubhaar, 2019). It is parallelized and offers many options to constrain the stochastic simulations such as continuous rotation/affinity maps or proportion targets. More details about the features of the DeeSse code are provided in Meerschman et al. (2013); Straubhaar et al. (2016, 2020)."
In Sections 4.2 and 4.3 there is a reference to probabilistic models. Confusing, and some clarification is required.	We are sorry that this was confusing. It's true that we do not compute probabilities during the simulation step. But the models are probabilistic. Not computing the probabilities is a technical trick. It does not mean that there is no underlying stochastic process and probabilities.
	To try to clarify, in addition to the new references that are provided, we propose to add a sentence explaining that DeeSse is used to generate an ensemble of realizations from which one can estimate any relevant probabilities for the problem of interest :
	"More details about the features of the DeeSse code are provided in Meerschman et al. (2013); Straubhaar et al. (2016, 2020). By generating an ensemble of realizations, it is then possible to estimate any probability of interest from the different facies maps."
5. At the top of Section 4.2, the authors state as follows: "Simulating a large number of realizations enables us to calculate probability maps". That is obviously true: when you generate multiple realizations, you can compute probabilities. Question is: what is the connection between these probabilities, on one hand, and uncertainty and risk, on the other? The authors need to make a convincing case that they model uncertainty accurately. Without it, they can only say that they can generate images.	This is a very interesting and important point that has led to heated discussions in the past and that will continue for sure to raise many discussions. The debate goes much beyond the context of this paper. The question of the reviewer revisits the debate about the subjectivist and frequentist interpretations of the notion of probability. This debate has involved mathematicians, philosophers, statisticians, etc. We do not think that it is reasonable to open this debate here since we will not be able to close it for sure.

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	In short, we consider that we are computing a probability that we interpret as subjectivist. It is a representation of our confidence in the model that we built and the amount of information that we have. We do not claim more than that.
	We think that the quality of the uncertainty estimation could be partly tested using cross-validation. This work is not presented in that paper, because our data set is too small and almost all of the models perform equally well (or bad) when there is little data available. If more data would be available, we could certainly compare the local accuracy and the calibration of the predictions of various stochastic models. We plan to do that in the future, but do not have the data for conducting that study yet. This is investigated in the paper currently submitted and under review by Juda P. : "Juda, P., Renard, P., & Straubhaar, J. (2020). A framework for the cross-validation of categorical geostatistical simulations"
	We still want to add a word of caution, local accuracy and calibration (meaning that we predict correctly the uncertainty on the facies at a certain location) do not necessarily mean that the connectivity of the sedimentary features is well honored and that the groundwater response of the model represents correctly the true one. Therefore, even if we use cross-validation and if performances are good, it may very well happen that the groundwater predictions are not.
	To summarize, we agree with the reviewer that the meaning of the estimated probability is an important issue that is not yet fully solved, but we tend to disagree with his last comment since we believe that such methods are useful to bring geological concepts in uncertainty estimations.
6. We need to see how the innovation (generating sedimentary patterns using a math/physical model) proposed in this study could make a difference. How would the generated images look like without the innovation? How does this innovation help in reducing uncertainty and improving accuracy?	The author raises again an interesting point, however, we do not think that the aim of this paper is to compare the MPS approach against other ones. Other publications have already compared MPS against SGS or pluri-Gaussian simulations and have shown the benefits of the multiple-point approach and its ability for

Some sort of cross-validation study(comparing	simulating complex and realistic patterns.
some sort of cross-validation study(comparing results obtained with and without the improvement) could be helpful.	The aim of this work is to present a new workflow that allows to generate complex non-stationary structures at a reservoir scale using MPS when little hard data are available. We propose to modify the introduction to better explain that objective.
	One of the novel ingredients of the proposed workflow is the computation of the trend using the solution of a diffusivity equation. We propose to extend the discussion about the advantage of this part of the method in the conclusion. The proposed text would be the following :
	"Solving numerically the diffusion equation allows to account easily for the complex geometry of the extension of the sedimentary basin when computing the trend map. Using that technique, it is straightforward to impose prescribed values of the trend on certain parts of the boundary and to ensure that the gradient of the trend will remain perpendicular to the sides of the domain."
	Regarding the advantage of using a trend map created from a math/physical model, we do not think that it would be useful to compare this approach against simulations that do not use a trend map. Indeed, it is well known from previous publications (eg. Chugunova and Hu, 2008) that using a non stationary training image without accounting for the trend creates some disordered patterns.
	Finally, as mentioned above and in the article, the cross-validation is an interesting aspect. But the lack of hard conditioning data makes its application difficult.
	It is planned in future work to acquire more data and to use cross validation to compare the performance of several geostatistical approaches. For the moment, we still believe that introducing the proposed workflow is interesting because it could be used by other researchers and adapted to their own studies.